ECLIPSE 300 (v2018.2) reservoir simulator with the CO2STORE module, Schlumberger

ECLIPSE 300 is a compositional finite-difference solver that is commonly used to simulate hydrocarbon production and has various other applications including carbon capture and storage modeling. The CO2STORE module accounts for the thermodynamic interactions between three phases: an H_2O-rich phase (i.e.,'liquid'), a CO_2-rich phase (i.e.,'gas'), and a solid phase, which is limited to several common salt compounds (e.g. NaCl, $CaCl_2$, and $CaCO_3$). Mutual solubilities and physical properties (e.g. density, viscosity, enthalpy, etc.) of the H_2O and CO_2 phases are calculated to match experimental results through a range of typical storage reservoir conditions, including temperature ranges between 12°C-100°C and pressures up to 60 MPa. Details of this method can be found in Spycher and Pruess (2005). Additional assumptions governing the phase interactions throughout the simulations are as follows:

- The salt components may exist in both the liquid and solid phases.

- The CO_2-rich phase (i.e.,'gas') density is obtained by using the Redlich-Kwong equation of state. The model was accurately tuned and modified as further described below (Redlich-Kwong, 1949).

- The brine density is first approximated as pure water then corrected for salt and CO_2 concentration by using Ezrokhi's method (Aseyev, 1992).

- The CO_2 gas viscosity is calculated per the methods described by Vesovic et al. (Fenghour, 1990).

The gas density was obtained using a modified Redlich-Kwong equation of state following a method developed by Spycher and Pruess, where the attraction parameter is made temperature dependent:

$$P = \left(\frac{RT_K}{V - b_{mix}}\right) - \left(\frac{a_{mix}}{T_K^{1/2}V(V + b_{mix})}\right)$$

where V is the molar volume, P is the pressure, T_K is the temperature in Kelvin, R is the universal gas constant, and a_{mix} and b_{mix} are the attraction and repulsion parameters.

The transition between liquid CO_2 and gaseous CO_2 can lead to rapid density changes of the gas phase; the simulator uses a narrow transition interval between the liquid and gaseous density to represent the two phase CO_2 region. With respect to time step selection, the software algorithm optimizes the time step duration based on specific convergence criteria designed to minimize numerical artifacts. For these simulations, time step size ranged from 8.64×10^1 to 4.32×10^6 seconds or 0.001 to 50 days. In all cases, the maximum solution change over a time step is monitored and compared with the specified target. Convergence is achieved once the model reaches the maximum tolerance where small changes of temperature and pressure calculation results occur on successive iterations. New time steps are chosen so that the predicted solution change is less than a specified target.

References

Aseyev, Z. a. (1992). *Ezrokhi's Method: Brine Density Approximated as Pure Water Corrected for Salt and CO2 Concentration* .

Fenghour, V. a. (1990). *CO2 Gas Viscosity.*

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Spycher, N., & Pruess, K. (2005). CO2-H2O mixtures in the geological sequestration of CO2.II. Partitioning in chloride brines at 12-100 C and up to 600 bar. *Geochimica et Cosmochimica Acta*, 69, No.13, 3309-3320.